Isoegomaketone

Inchi: InChI=1S/C10H12O2/c1-8(2)3-4-10(11)9-5-6-12-7-9/h3-8H,1-2H3/b4-3+
InchiKey: XEYCZVQIOJGCNL-ONEGZZNKSA-N
Formula: C10H12O2
SMILES: CC(C)C=CC(=O)c1ccoc1
Mol. weight [g/mol]: 164.20
CAS: 34348-59-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	2.675		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
ripol	1949.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34348599&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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